3.091 OCW Scholar

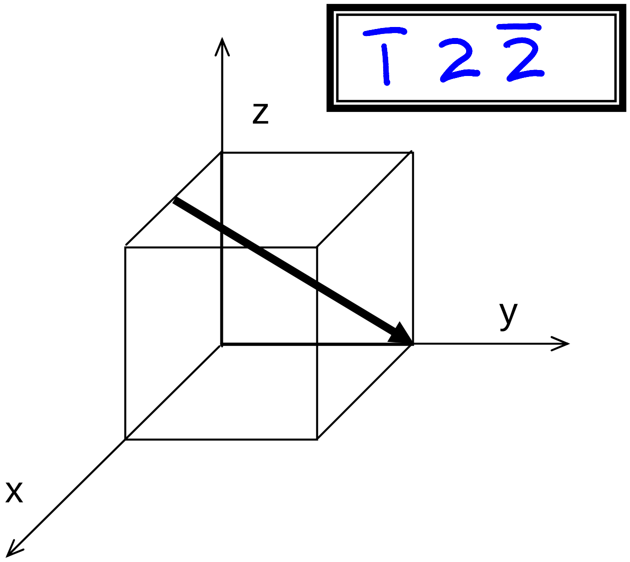
Self-Asessment

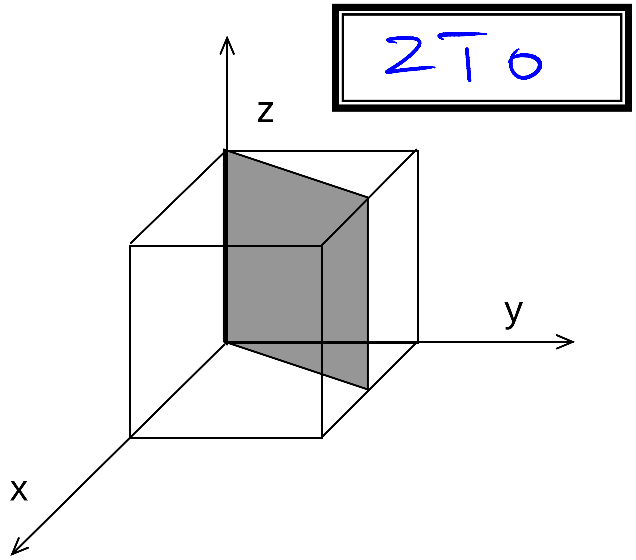
Crystalline Materials

Supplemental Exam Problems for Study

Solutions Key

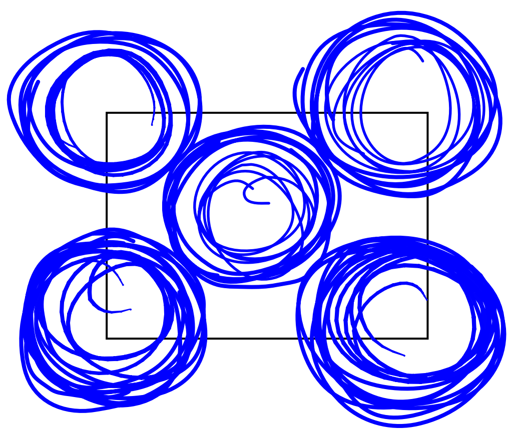
Problem #1





(a) Using proper crystallographic notation identify the direction (left) and the plane (right) depicted in the above sketches.

(b) Here is the (011) plane in a unit cell of lithium (Li). Indicate the positions of all atoms lying in the plane. Represent atoms as 2-dimensional slices of space-filling spheres.



Problem #2

(a) A crystal of iridium (Ir) is analyzed by x-ray diffraction through exposure to molybdenum K_α radiation, for which $\lambda_{K_\alpha} = 0.721$ Å $= 7.21 \times 10^{-11}$ m. Calculate the angle of reflection, θ, of the lowest-index plane present in the diffractogram. The lattice constant of Ir, *a*, is 3.84 Å.

$\lambda = 2d\sin\theta$

$\therefore \theta = \sin^{-1}\dfrac{\lambda}{2d}$

Ir is FCC

$\therefore$ lowest index plane

is $(111) \Rightarrow d_{111} = \dfrac{a}{\sqrt{3}}$

$\rightarrow \theta = \sin^{-1}\dfrac{\lambda\sqrt{3}}{2a}$

$= \sin^{-1}\dfrac{0.721 \times \sqrt{3}}{2 \times 3.84} = 9.36°$

(b) If you wanted to increase the angle at which the reflection described in part (a) is observed, would you replace the Mo target with a silver (Ag) target or a copper (Cu) target? Explain the reasoning behind your choice.

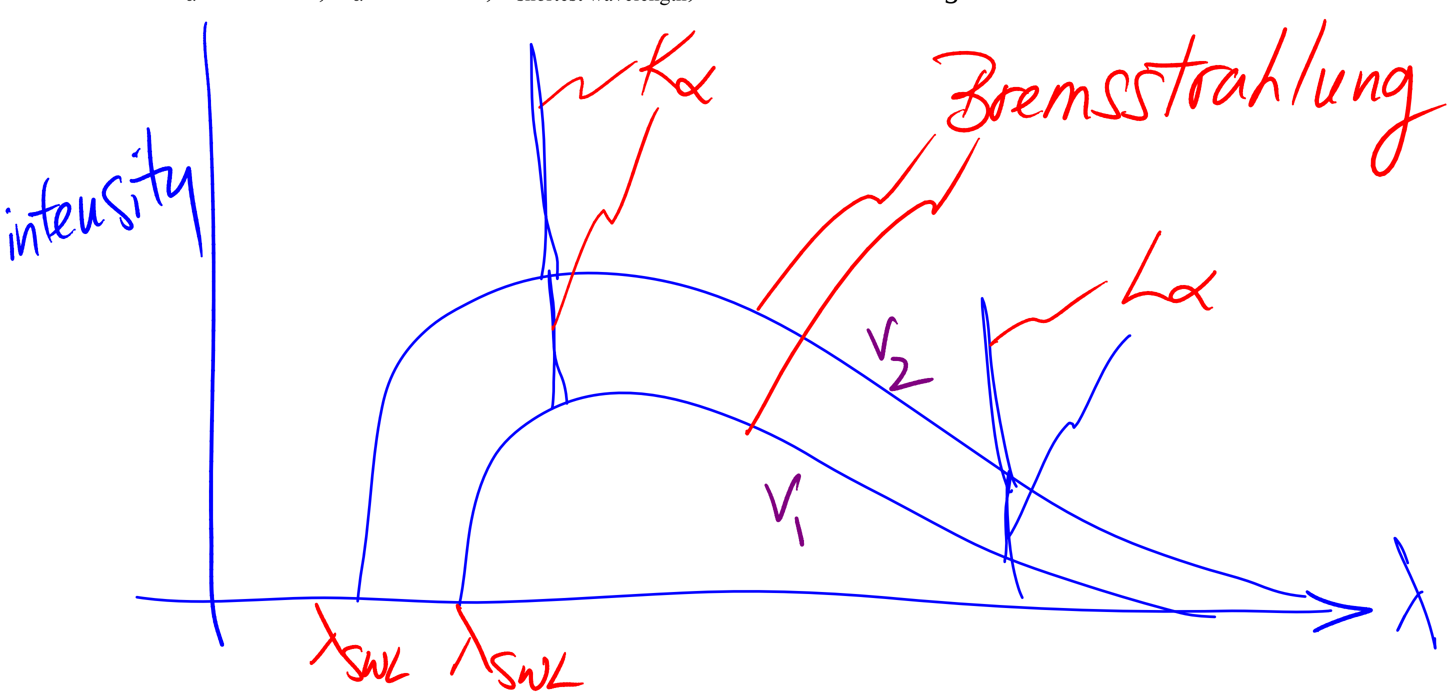
$\lambda = 2d\sin\theta$

if d constant $\Rightarrow \theta\uparrow$ if $\lambda\uparrow$

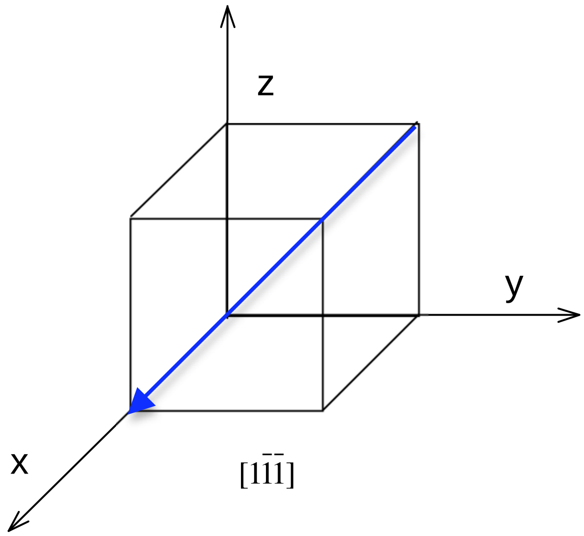
from Moseley's Law $\nu = \dfrac{1}{\lambda} \propto (Z-\sigma)^2$

$\therefore \lambda\uparrow$ when $Z\downarrow$ $\therefore$ choose Cu

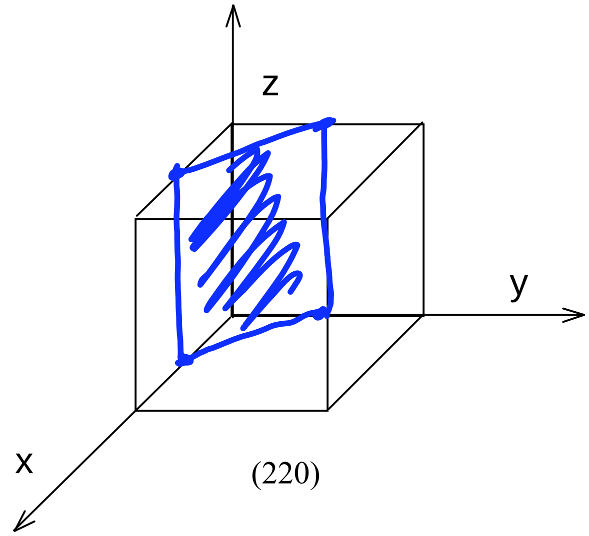
(c) In one drawing, sketch the emission spectra (**intensity** *versus* **wavelength**) of an x-ray tube operated at each of two different values of plate voltage, V_1 and V_2, where $V_2 > V_1 >$ the threshold voltage to generate the characteristic lines. On each spectrum in your sketch, label the features associated with K_α radiation, L_α radiation, $\lambda_{\text{shortest wavelength}}$, and *Bremsstrahlung*.



Problem #1



$[1\bar{1}\bar{1}]$



(220)

(a) For each unit cell above, draw the crystallographic feature indicated and label it clearly.

(b) Urbium (Ub) is an upscale element found in large cities. Its unit cell is cubic. Using the values of its molar volume and lattice constant, determine the crystal structure of Ub.

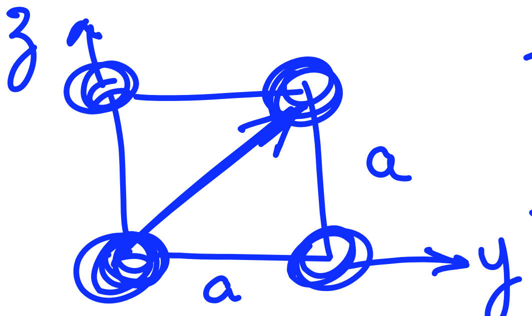
DATA: molar volume, V_{mol} = 9.41 cm^3/mol lattice constant, a = 3.15 Å = 3.15×10^{-8} cm

$$\frac{n}{a^3} = \frac{N_{AV}}{V_m} \therefore n = \frac{a^3 N_{AV}}{V_m} = \frac{(3.15\times10^{-8})^3\ 6.02\times10^{23}}{V_m}$$

$$= 2$$

$$\therefore BCC$$

(c) Calculate the linear density of atoms along [011] in lithium (Li). The value of the lattice constant in Li is 3.51 Å. Express your answer in units of atoms /Å.



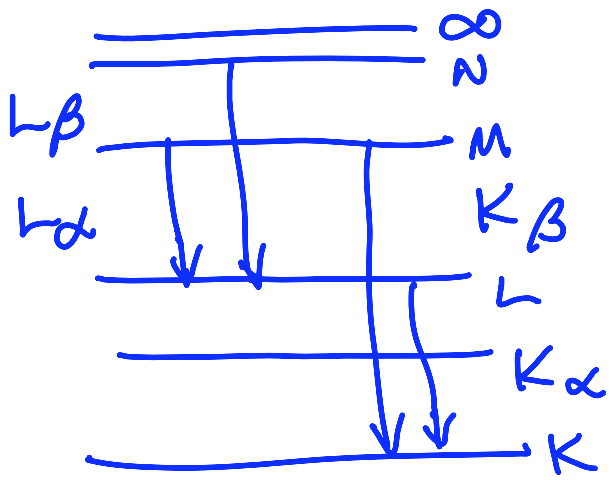
$$2 \times \frac{1}{2} \text{ atom} / \sqrt{2}a$$

$$\frac{2}{a^3} = \frac{N_{AV}}{V_m} \Rightarrow a = \left(\frac{2V_m}{N_{AV}}\right)^{1/3} = 3.51\times10^{-8}\ cm$$

$$\therefore \frac{1}{\sqrt{2}a} = \frac{1}{\sqrt{2}\times3.5} = 0.201 \text{ atom}/Å$$

Problem #2

(a) Draw the energy-level diagram of the target (anode) of an x-ray tube operating at a plate voltage great enough to generate the characteristic lines. Indicate the features associated with emission of ❶ K_α, ❷ K_β, ❸ L_α, and ❹ L_β radiation. The drawing need not be to scale but should reflect qualitative distinctions in magnitudes of transition energies.



(b) ***Estimate*** the energy of the transition associated with the generation of K_β radiation from a target made of silver (Ag). The values of the screening factor, σ, are 1 for K_α and 7.4 for L_α.

$$\Delta E_{K_\beta} = E_3 \rightarrow E_1 = E_3 \rightarrow E_2 + E_2 \rightarrow E_1$$

use Mosely's Law

$$\bar{\nu}_{3\to2} = \frac{5}{36} R (47-7.4)^2 = 2.40 \times 10^9 \qquad \Delta E = hc\bar{\nu}$$

$$\bar{\nu}_{2\to1} = \frac{3}{4} R (47-1)^2 = 1.75 \times 10^{10} \qquad = hc(2.40 \times 10^9 + 1.75 \times 10^{10})$$

$$= 6.6 \times 10^{-34} \times 3 \times 10^8 \times (\quad) = 3.93 \times 10^{-15}\ \mathrm{J}$$

(c) A sample of chromium (Cr) is analyzed by x-ray diffraction using copper K_α radiation for which λ_{K_α} = 1.5418 Å. Determine the Miller indices of the plane from which the angle of reflection, θ, is 31.4°. The lattice constant of Cr, *a*, is 2.96 Å. Report your answer in the form (*hkl*).

$$\lambda = 2d\sin\theta \qquad d = \frac{a}{(h^2+k^2+l^2)^{1/2}}$$

$$\therefore \lambda = \frac{2a\sin\theta}{(h^2+k^2+l^2)^{1/2}}$$

$$\therefore h^2+k^2+l^2 = \frac{4a^2\sin^2\theta}{\lambda^2} = \frac{4 \times (2.96)^2 \sin^2(31.4°)}{(1.5418)^2} = 4.00$$

Cr is BCC

∴ hkl that gives

$h^2+k^2+l^2 = 4$ ✓

(002)

Problem #1

The dominant defect in zirconia (ZrO_2) is the Schottky disorder.

(a) Write the reaction that represents the formation of a Schottky defect in ZrO_2.

$$null = V_{Zr}^{''''} + 2V_O^{\bullet\bullet}$$

(b) Calculate the fraction of vacant zirconium sites in a crystal of ZrO_2 at a temperature of 333 K. The enthalpy of Schottky defect formation, ΔH_S, has a value of 2.1 eV / defect, and the entropic prefactor, A, has a value of 3.091.

$$f_v = A\exp - \frac{\Delta H_S}{k_B T} = 3.091\exp - \frac{2.1 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23} \times 333} = 5.44 \times 10^{-32}$$

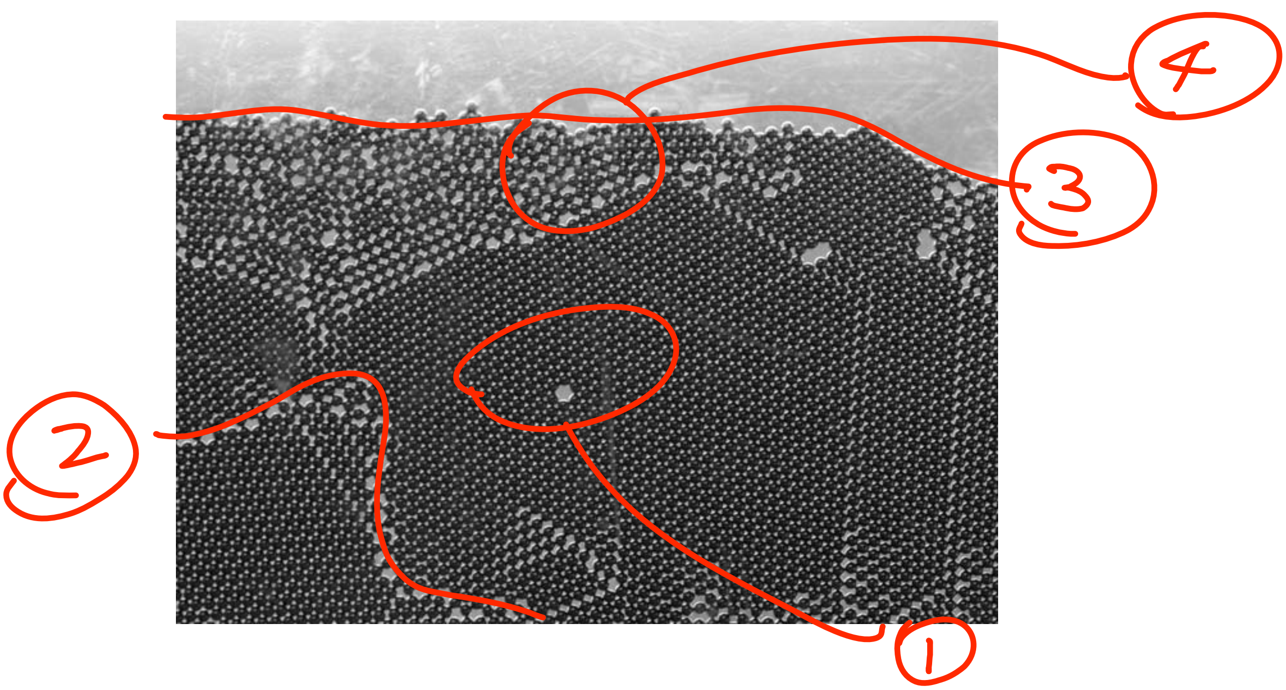
$n_S = n_{Zr}$ vacancies

(c) To increase the population of oxide vacancies ZrO_2 can be doped with calcia (CaO). Write the reaction showing that for each CaO that is incorporated into the ZrO_2 crystal an oxide vacancy is formed.

$$CaO \xrightarrow{ZrO_2} Ca_{Zr}^{''} + O_O^{x} + V_O^{\bullet\bullet}$$

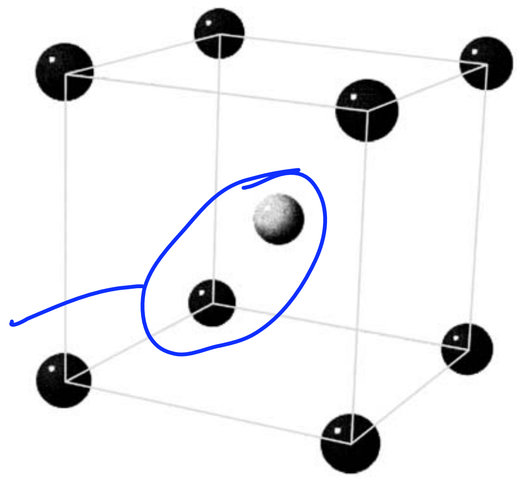
(d) The figure below is an image of the ATOMIX™ kinetic sculpture that was shown in lecture. The device consists of a layer of stainless steel ball bearings free to roll about between two plates of poly(methyl methacrylate) (PMMA). The balls can be thought of as atoms in a two-dimensional likeness of a solid composed of atoms bearing no net charge, e.g., a metal. For each of the following, mark directly on the image one feature that would serve as a two-dimensional representation:

(1) vacancy; (2) grain boundary; (3) free surface; (4) amorphous region.



Problem #2

The crystal structure of cesium chloride (CsCl) is shown in the adjacent figure. The dark spheres represent atoms of Cl.



basis

(a) Name the crystal system.

cubic

(b) Name the Bravais lattice.

Simple Cubic

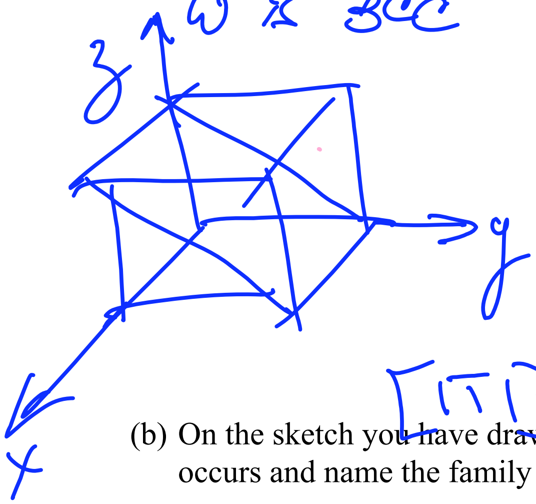
(c) Name the basis of the crystal structure and indicate the basis by markup of the figure.

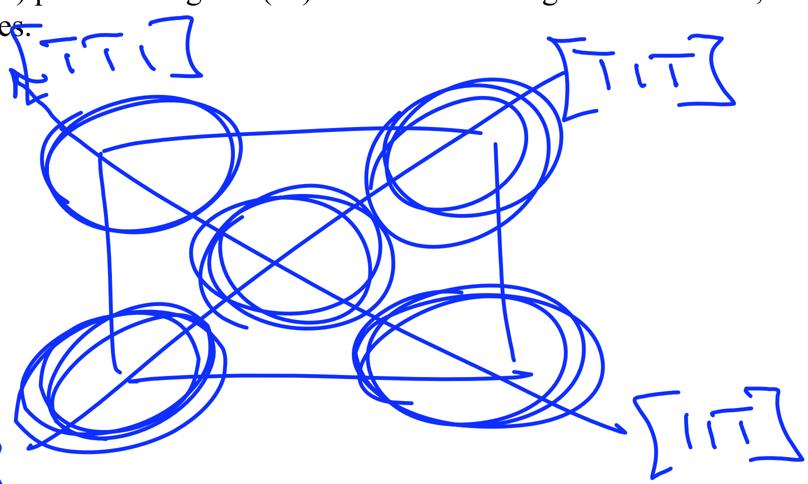
Cl^- & Cs^+

Problem #3

(a) Sketch a fragment of the (011) plane in tungsten (W) to show the arrangement of atoms, which are to be represented as hard spheres.

W is BCC





(b) On the sketch you have drawn in answer to part (a), draw and label all directions along which slip occurs and name the family of directions to which they belong.

(c) Calculate the atomic packing density in the (011) plane of W. Express your answer in units of atoms cm^{-2}.

no. atoms / cell $= (4 \times 1/4) + 1 = 2$

area of cell $= a \times \sqrt{2}a = \sqrt{2}a^2$

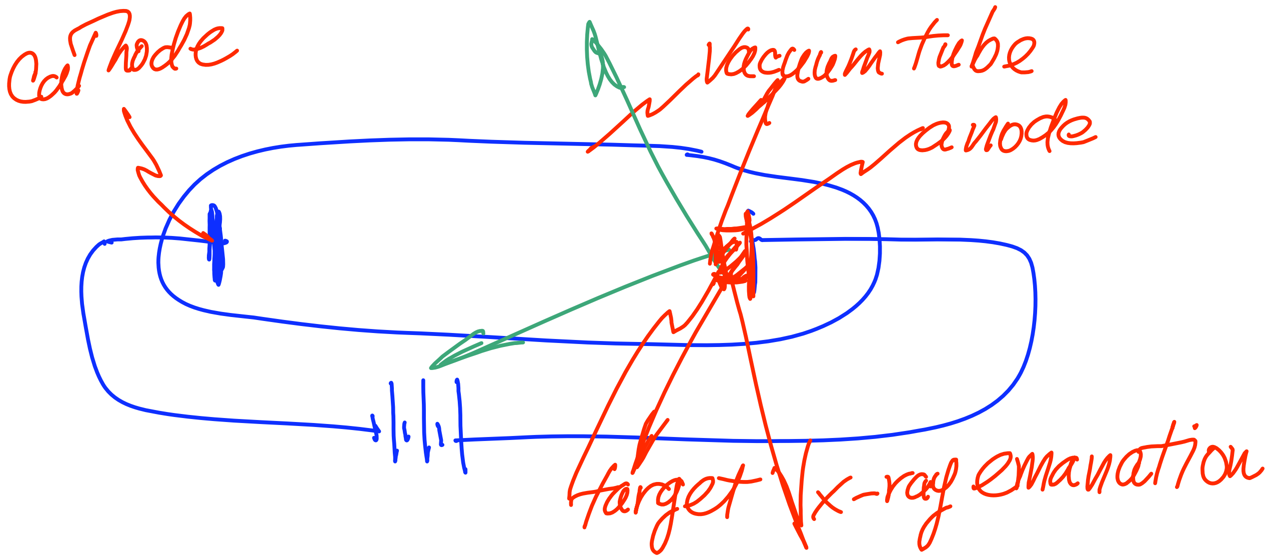
for BCC $\frac{2}{a^3} = \frac{N_{AV}}{V_{molar}} \Rightarrow a = \left(\frac{2 V_{molar}}{N_{AV}}\right)^{1/3} = \left(\frac{2 \times 9.50}{6.02 \times 10^{23}}\right)^{1/3}$

$= 3.16 \times 10^{-8}$ cm

$\therefore$ density $= \frac{2}{\sqrt{2}a^2} = \frac{\sqrt{2}}{(3.16 \times 10^{-8})^2} = 1.42 \times 10^{15}$ atoms/cm^2

Problem #9

(a) Draw a cartoon depicting the device that generates x-rays. Label the following features: vacuum tube, cathode, anode, target. Indicate on your drawing the emanation of x-rays.



(b) Röntgen's gas discharge tube was highly inefficient and unsafe. Among the modifications made by William D. Coolidge (MIT class of 1896), were the following: ❶ vacuum tube instead of tube containing gas; and ❷ water cooled anode. Describe how each modification represents an improvement over Röntgen's device. In your answer specify the problem addressed by the modification and explain how the modification overcomes the problem.

❶ electrons collided w/ gas molecules/atoms ⇒ loss of efficiency ⇒ vacuum tube eliminates the problem —

❷ energy of ballistic electrons heated the target & anode so the tube needed to be operated intermittently ⇒ with water cooling, tube could run continuously.

(c) The Duane-Hunt Law calculation gives a value of 0.666 Å (6.66×10^{-11} m) for the shortest wavelength produced by an x-ray tube. What must be the value of the plate voltage under these circumstances?

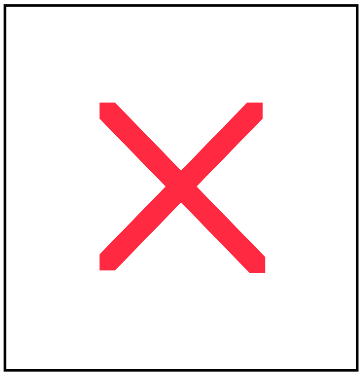
$$\lambda = \frac{12400}{V} \quad \therefore \quad V = \frac{12400}{\lambda} = \frac{12400}{0.666}$$

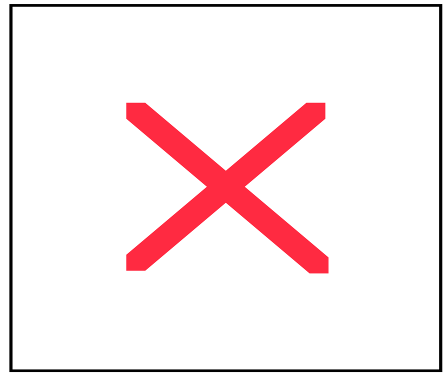
$$= 1.86 \times 10^{4}\ V$$

$$= 18.6\ kV$$

Problem #10

Give the rotational symmetry of each of the following patterns. Express your answer as *n*-fold.





❶ 4-fold

❷ 3-fold

❸ 1-fold